## An asymptotic solution for the SHE equations describing the charge transport in semiconductors.

#### SALVATORE FABIO LIOTTA

Dipartimento di Matematica e Informatica, Università di Catania Viale A. Doria 6, 95125, Catania, Italy

**Abstract** In this paper an asymptotic solution of the spherical harmonics equations describing the charge transport in semiconductors is found. This solution is compared with a numerical solution for bulk silicon device. We also indicate application of this solution to the construction of high field hydrodynamical models.

Keywords Semiconductors, Boltzmann equation, Spherical harmonics expansion.

#### 1 Introduction.

In the framework of charge transport in semiconductors, a technique widely used in order to find approximate solutions of the Boltzmann transport equation (BTE) is based on a spherical harmonics expansion (SHE) of the distribution function (Rahmat, White and Antoniadis, 1996; Vecchi and Rudan, 1998; Ventura, Gnudi and Baccarani, 1995; Liotta and Struchtrup, 2000). Recently an asymptotic solution of the SHE equations was found (Liotta and Majorana, 1999) in the case of a homogeneous (bulk) device with a simple parabolic band structure. Despite the very simple situation in which this solution was obtained, it has revealed to be very useful in order to develop new asymptotic hydrodynamical models describing the hot electron population in silicon devices (both in the homogeneous and non-homogeneous case). In particular see Anile and Mascali (2000) and Anile, Liotta and Mascali (2000), where this asymptotic solution was used in order to close the set of moment equations.

The aim of this work is to show the possibility of finding a new asymptotic solution generalizing that derived in Liotta and Majorana (1999) to the case of a non-parabolic band structure (Kane model). this solution reduces to the old one when the non-parabolicity parameter goes to zero. The importance is due to the fact that the Kane equation fits better the real band structure in the high field regime. Therefore this solution can be very useful in order to develop improved high field hydrodynamical models which could describe better the hot electron population. This solution is also interesting by itself in the framework of SHE models.

## 2 Basic equations.

We consider the case of unipolar semiconductor devices in which the current is essentially due to electrons (but the results can be generalized to holes). The semiclassical description of the electron transport is based on the BTE (Markowich et al., 1990; Ferry, 1991; Cercignani, 1987), which writes

$$\frac{\partial f}{\partial t} + \mathbf{v}(\mathbf{k}) \cdot \nabla_{\mathbf{x}} f - \frac{\mathbf{e}}{\hbar} \mathbf{E} \cdot \nabla_{\mathbf{k}} f = Q(f), \qquad (1)$$

here  $f(t, \mathbf{x}, \mathbf{k})$  is the electron distribution function, generally depending on time t, position  $\mathbf{x}$  and wave vector  $\mathbf{k}$  (belonging to the first Brillouin zone B).  $\mathfrak{e}$  is the absolute

value of the electron charge,  $\hbar$  the reduced Planck constant,  $\mathbf{E}$  the electric field.  $\nabla_{\mathbf{x}}$  and  $\nabla_{\mathbf{k}}$  denote the gradient with respect to  $\mathbf{x}$  and  $\mathbf{k}$  respectively. The group velocity  $\mathbf{v}(\mathbf{k})$  is determined by the conduction band structure:  $\mathbf{v}(\mathbf{k}) = \frac{1}{\hbar} \nabla_{\mathbf{k}} \varepsilon(\mathbf{k})$ , where  $\varepsilon(\mathbf{k})$  is the electron energy which depends on the wave vector. Q is the collision operator which in the non-degenerate case has the form

$$Q(f) = \int W(\mathbf{k}, \tilde{\mathbf{k}}) f(t, \mathbf{x}, \tilde{\mathbf{k}}) d\tilde{\mathbf{k}} - f(t, \mathbf{x}, \mathbf{k}) \int W(\tilde{\mathbf{k}}, \mathbf{k}) d\tilde{\mathbf{k}},$$
(2)

 $W(\mathbf{k}, \tilde{\mathbf{k}})$  representing the electron scattering rate from a state with wave vector  $\tilde{\mathbf{k}}$  to one with wave vector  $\mathbf{k}$ .

We will consider a stationary and homogeneous situation (bulk device), neglecting the Poisson equation and taking into account only a constant externally applied electric field, then it will be  $f = f(\mathbf{k})$ . Moreover, we will suppose that the electric field is directed along the  $\mathbf{x}$ -axis so to have a cylindrical symmetry around this axis and represent the two-dimensional momentum space by means of the polar coordinates  $k = |\mathbf{k}| (= \xi(\varepsilon))$  and  $\theta = \arccos(\mathbf{k} \cdot \mathbf{k}_x/|\mathbf{k}||\mathbf{k}_x|)$ , where  $\mathbf{k}_x$  is the projection of  $\mathbf{k}$  along x. Therefore the distribution function can be expanded in Legendre polynomials of the angle  $\theta$  (Rahamat et al., 1996; Liotta and Struchtrup, 2000)

$$f(\mathbf{k}) = \sum_{n} f_n(\varepsilon) P_n(\cos \theta),$$
 (3)

where  $P_n$  is the *n*th order Legendre polynomial. This expansion will be computationally viable only if few spherical harmonics are enough to accurately represent the momentum space distribution. We will assume that the first two terms of the previous expression give a good approximation

$$f(\mathbf{k}) \simeq f_0(\varepsilon) + f_1(\varepsilon) \cos \theta$$
. (4)

The lowest order harmonic coefficient furnishes information about the isotropic part of the distribution function and  $\int f_0 d\mathbf{k}$  yields the electron concentration. The first order harmonic coefficient describes the asymmetry of the distribution function in the direction of the applied electric field, and  $\int f_1 \cos \theta \mathbf{v}(\mathbf{k}) d\mathbf{k} / \int f_0 d\mathbf{k}$  gives the hydrodynamical velocity of the electron gas.

We will assume a spherically symmetric band structure of the Kane form (Ferry, 1991, Jacoboni and Lugli, 1989; Tomizawa, 1993)

$$\gamma(\varepsilon) := \varepsilon(1 + \alpha\varepsilon) = \frac{\hbar^2 k^2}{2m^*},\tag{5}$$

where  $m^*$  is the electron effective mass and  $\alpha$  the constant non-parabolicity parameter. By putting  $\alpha=0$  one obtains the usual parabolic band approximation. With this choice we can assume for the first Brillouin zone  $B\equiv\mathbb{R}^3$  and we have  $\mathbf{v}(\mathbf{k})=\frac{\hbar\mathbf{k}}{m^*(2\alpha\varepsilon+1)}$ .

As regards collisions, we will take into account the interaction between electrons and non-polar optical phonons and that between electrons and acoustical phonons, the latter in the elastic approximation, valid when the thermal energy is much greater than that of the phonon involved in the scattering. We consider the electron scatterings with ionized impurities to be negligible, *i.e.* we assume the doping density to be low. Then the transition rate of the collision operator reads (Jacoboni and Lugli, 1989; Tomizawa, 1993)

$$W(\mathbf{k}, \tilde{\mathbf{k}}) = \mathcal{K}_{op} \left[ n_{op} \ \delta(\varepsilon - \tilde{\varepsilon} - \hbar \omega_{op}) + (n_{op} + 1) \ \delta(\varepsilon - \tilde{\varepsilon} + \hbar \omega_{op}) \right] + \mathcal{K}_{ac} \delta(\varepsilon - \tilde{\varepsilon}), \quad (6)$$

where  $\varepsilon = \varepsilon(\mathbf{k})$ ,  $\tilde{\varepsilon} = \varepsilon(\tilde{\mathbf{k}})$ ,  $n_{op} = \left(\exp\left(\frac{\hbar\omega_{op}}{k_BT_L}\right) - 1\right)^{-1}$  is the thermal equilibrium optical phonon number and  $\mathcal{K}_{op}$  and  $\mathcal{K}_{ac}$  are respectively the non-polar optical and acoustical kernel coefficients (constant at a first approximation).  $\hbar\omega_{op}$  is the optical phonon energy,  $k_B$  the Boltzmann constant and  $T_L$  the lattice temperature. These choices are appropriate for silicon devices.

The SHE equations are easily obtained by inserting the expansion (3) into the BTE (1) and balancing the terms of the same order in  $P_n(\cos \theta)$ . To generate a closed set of equations, all coefficients of order higher than the first are set to be zero, see Rahmat et al. (1996) (a closure inspired by the Grad moment method, see Grad, 1958).

But for the aims of this paper it is preferable to perform a change of variables and write down a set of two coupled equations in the unknowns

$$N(\varepsilon) = \sigma(\varepsilon) f_0(\varepsilon), \tag{7}$$

$$P(\varepsilon) = \frac{8}{3} \pi \frac{\sqrt{m^*}}{\hbar^3} \gamma(\varepsilon) f_1(\varepsilon), \qquad (8)$$

where

$$\sigma(\tilde{\varepsilon}) := \int_{\mathbb{R}^3} \delta(\varepsilon(\mathbf{k}) - \tilde{\varepsilon}) \, d\mathbf{k} = 4\sqrt{2}\pi \left(\frac{\sqrt{m^*}}{\hbar}\right)^3 H(\tilde{\varepsilon})(\gamma(\tilde{\varepsilon}))^{\frac{1}{2}} \, \gamma'(\tilde{\varepsilon}) \tag{9}$$

is the density of states .  $H(\varepsilon)$  is the Heaviside step function and  $\gamma'(\varepsilon) \equiv \frac{d\gamma}{d\varepsilon} = (1+2\alpha\varepsilon)$ . So doing, the expansion (4) writes

$$f(\mathbf{k}) \simeq \frac{N(\varepsilon)}{\sigma(\varepsilon)} + \left(\frac{8}{3}\pi \frac{\sqrt{m^*}}{\hbar^3} \gamma(\varepsilon)\right)^{-1} P(\varepsilon) \cos \theta.$$

These new variables have also a direct physical interpretation:

$$\int_{0}^{+\infty} N(\varepsilon) d\varepsilon = \int_{\mathbb{R}^{3}} f_{0}(\varepsilon) d\mathbf{k} \quad , \quad \int_{0}^{+\infty} P(\varepsilon) d\varepsilon = \int_{\mathbb{R}^{3}} v(\varepsilon) f_{1}(\varepsilon) d\mathbf{k}, \quad (10)$$

 $(v(\varepsilon) = |\mathbf{v}_x|)$  and are very suitable for our problem.

With these choices the equations of our SHE model, in the stationary homogeneous case, write:

$$-\mathfrak{e}E\frac{dP}{d\varepsilon} = G_1(N) \tag{11}$$

$$-\mathfrak{e}E\frac{d(g(\varepsilon)N)}{d\varepsilon} + \mathfrak{e}Eh(\varepsilon)N = G_2(P)$$
(12)

where

$$G_{1}(N) = \mathcal{K}_{op}\sigma(\varepsilon) \left[ (n_{op} + 1)N(\varepsilon + \hbar\omega_{op}) + n_{op}N(\varepsilon - \hbar\omega_{op}) \right] - \mathcal{K}_{op} \left[ n_{op}\sigma(\varepsilon + \hbar\omega_{op}) - (n_{op} + 1)\sigma(\varepsilon - \hbar\omega_{op}) \right] N(\varepsilon),$$

$$G_{2}(P) = - \left[ n_{op}\mathcal{K}_{op}\sigma(\varepsilon + \hbar\omega_{op}) + (n_{op} + 1)\mathcal{K}_{op}\sigma(\varepsilon - \hbar\omega_{op}) + \mathcal{K}_{ac}\sigma(\varepsilon) \right] P(\varepsilon)$$

and

$$g(\varepsilon) := \frac{2}{3} \frac{\gamma(\varepsilon)}{m^* (\gamma'(\varepsilon))^2} \quad , \quad h(\varepsilon) := \frac{1}{m^* \gamma'(\varepsilon)} - \frac{4}{3} \frac{\alpha}{m^*} \frac{\gamma(\varepsilon)}{(\gamma'(\varepsilon))^3}.$$

We would like to underline that equations (11)-(12) can be obtained directly from the BTE by using a new alternative procedure. It consists in multiplying both sides of

equation (1) respectively by  $\delta(\varepsilon(\mathbf{k}) - \tilde{\varepsilon})$  and by  $\mathbf{v}(\mathbf{k})\delta(\varepsilon(\mathbf{k}) - \tilde{\varepsilon})$  and then formally integrating with respect to  $\mathbf{k}$  over the whole space  $\mathbb{R}^3$ . Some suitable closure relations are needed: in particular by assuming that f depends on  $\mathbf{k}$  only through the variable  $\varepsilon$  one obtains equations (11)-(12) in the general non-homogeneous, non-stationary case (Liotta and Majorana, 1999; Majorana, 1998). This method is similar to the method of frequency dependent moments of radiation hydrodynamics (Thorne, 1981).

#### 3 Dimensionless equations and physical parameters.

It is useful to introduce dimensionless variables: let

$$t_* := \left[ 4\sqrt{2}\pi \left( \frac{\sqrt{m^*}}{\hbar} \right)^3 \sqrt{k_B T_L} \mathcal{K}_{op} n_{op} \right]^{-1}, \quad \ell_* := \left( \frac{k_B T_L}{m^*} \right)^{\frac{1}{2}} t_*, \quad \varepsilon_* := k_B T_L,$$

$$w := \frac{\varepsilon}{\varepsilon_*}, \quad n(w) := u_* \ell_*^3 N(\varepsilon), \quad p(w) := u_* \ell_*^2 t_* P(\varepsilon),$$

$$\lambda := \frac{\hbar \omega_{op}}{k_B T_L}, \quad a := \frac{n_{op} + 1}{n_{op}} = e^{\lambda}, \quad \kappa := \frac{\mathcal{K}_{ac}}{n_{op} \mathcal{K}_{op}}, \quad \zeta := \mathfrak{e} E \frac{\ell_*}{u_*}, \quad \beta := \alpha \ \varepsilon_*.$$

Moreover in the following we put  $\chi(w) := w(1 + \beta w)$  and  $\chi'(w) \equiv \frac{d\chi}{dw} = (1 + 2\beta w)$ . By using these new variables, equations (11)-(12) become

$$-\zeta \frac{dp}{dw} = \mu(w) \left[ an(w+\lambda) + n(w-\lambda) \right] - \left[ \mu(w+\lambda) + a\mu(w-\lambda) \right] n(w) \tag{13}$$

$$\zeta \left[ -\frac{d(r(w)n)}{dw} + q(w)n \right] = -\left[ \mu(w+\lambda) + a\mu(w-\lambda) + \kappa\mu(w) \right] p(w) \tag{14}$$

where

$$\mu(w) := H(w) [\chi(w)]^{\frac{1}{2}} \chi'(w)$$

$$r(w) := \frac{2}{3} \frac{\chi(w)}{[\chi'(w)]^2}$$

$$q(w) := \frac{1}{\chi'(w)} - \frac{4}{3} \beta \frac{\chi(w)}{[\chi'(w)]^3}.$$

We associate the following conditions to equations (13)-(14)

$$\begin{split} n(0) &= 0 \ (\Rightarrow p(0) = 0) \,, \qquad \lim_{w \to +\infty} p(w) = 0 \\ n(w) &\geq 0 \quad \forall \ w \geq 0 \,, \qquad \int_0^{+\infty} n(w) \, dw > 0 \quad and \quad < +\infty \,. \end{split}$$

Since equations (13)-(14) are linear and homogeneous, if a solution (n(w), p(w)), satisfying the above conditions exists, then, for every c > 0, also (cn(w), cp(w)) is a solution. The appropriate values of the physical parameters, in the case of a silicon device, are given in table I, were  $m_e$  denotes the electron rest mass.

$m^* = 0.32  m_e$	$T_L = 300 \text{ K}$	$\hbar\omega_{op} = 0.063 \text{ eV}$
$\mathcal{K}_{op} = \frac{(D_t K)^2}{8\pi^2 \rho \omega_{op}}$	$D_t K = 11.4 \text{ eV } \mathring{A}^{-1}$	$\rho=2330~\rm Kg~m^{-3}$
$\mathcal{K}_{ac} = \frac{k_B T_L}{4\pi^2 \hbar v_0^2 \rho} \Xi_d^2$	$\Xi_d = 9 \text{ eV}$	$v_0 = 9040 \text{ m sec}^{-1}.$
$\alpha = 0.5  eV^{-1}$		

**Table I.** Values of the physical parameters used in this paper.

Using these parameters, we get  $\lambda \simeq 2.437$ ,  $\kappa \simeq 5.986$  and  $\beta \simeq 0.012926$ .

## 4 Asymptotic equations.

Now we want to show that it is possible to find an approximate solution of the equations (13)-(14) valid for high values of the electron energy.

It is useful to introduce a new variable  $\psi(w)$  defined by

$$n(w) = \mu(w)\psi(w). \tag{15}$$

Equations (13)-(14) become

$$-\zeta \frac{dp}{dw} = \mu(w) \left[ a\mu(w+\lambda)\psi(w+\lambda) + \mu(w-\lambda)\psi(w-\lambda) \right] - \mu(w) \left[ \mu(w+\lambda) + a\mu(w-\lambda) \right] \psi(w)$$
(16)

$$\frac{2}{3}\zeta \frac{\left[\chi(w)\right]^{\frac{3}{2}}}{\chi'(w)} \frac{d\psi}{dw} = -\left[\mu(w+\lambda) + a\mu(w-\lambda) + \kappa\mu(w)\right]p(w). \tag{17}$$

Because we look for an asymptotic form of the equations (16)-(17) for large values of the energy w, we expand the coefficients of the equations up to the zeroth order in  $\lambda$ :  $\mu(w \pm \lambda) \simeq \mu(w)$ . In this way we obtain a new set of equations

$$-\zeta \frac{dp_A}{dw} = \mu^2(w) \left[ a\psi_A(w+\lambda) + \psi_A(w-\lambda) - (a+1)\psi_A(w) \right]$$
 (18)

$$p_A(w) = \frac{2}{3} \zeta \frac{[\chi(w)]^{\frac{3}{2}}}{\chi'(w)\mu(w) [1+a+\kappa]} \frac{d\psi_A}{dw}, \tag{19}$$

where the subscript A label the new unknowns. Substituting (19) into (18), it follows

$$-\frac{2}{3}\frac{\zeta^{2}}{(1+a+\kappa)}\left[\frac{\chi(w)}{[\chi'(w)]^{2}}\psi''_{A} + \left(\frac{1}{\chi'(w)} - \frac{4\beta\chi(w)}{[\chi'(w)]^{3}}\right)\psi'_{A}\right] = \chi(w)\left[\chi'(w)\right]^{2}\left(a\psi_{A}\left(w+\lambda\right) + \psi_{A}\left(w-\lambda\right) - (a+1)\psi_{A}\left(w\right)\right),\tag{20}$$

where the primes denote derivatives with respect to w.

#### 5 Approximate solution.

In order to find an approximate solution of equation (20) we expand the coefficients up to the first order in the non-parabolicity parameter  $\beta$ .

$$-\frac{2}{3}\frac{\zeta^{2}}{(1+a+\kappa)}\left[\left(w-3\beta w^{2}\right)\psi_{A}''+\left(1-6\beta w\right)\psi_{A}'\right]=\left(w+5\beta w^{2}\right)\left(a\psi_{A}\left(w+\lambda\right)+\psi_{A}\left(w-\lambda\right)-\left(a+1\right)\psi_{A}\left(w\right)\right).$$
(21)

This choice is justified by the smallness of  $\beta$  and by the Kane equation itself, which is of the first order in the non-parabolicity parameter.

We will search for solutions of equation (21) having the form

$$\psi_A(w) = e^{f(w)}$$
, with  $f(w) := \eta_0 w + \eta_1 \beta w^2$ , (22)

where  $\eta_0$  and  $\eta_1$  are functions of the applied electric force  $\zeta$ .

It is useful to observe that  $f(w \pm \lambda) = f(w) + f(\pm \lambda) \pm 2\eta_1 \beta \lambda w$ . Expanding the following quantities up to the first order in  $\beta$ :

$$e^{\pm 2\eta_1 \beta \lambda w} \simeq 1 \pm 2\eta_1 \beta \lambda w,$$
  
 $e^{f(\pm \lambda)} \simeq e^{\pm \eta_0 \lambda} \left( 1 + \eta_1 \lambda^2 \beta \right),$ 

substituting (22) into (21) and retaining only terms up to first order in  $\beta$ , we obtain, after dropping the common factor  $e^{f(w)}$ , the equation

$$-\frac{2}{3} \frac{\zeta^{2}}{(1+a+\kappa)} \left[ \eta_{0} + \left( \eta_{0}^{2} + 4\beta\eta_{1} - 6\beta\eta_{0} \right) w + \left( -3\beta\eta_{0}^{2} + 4\beta\eta_{0}\eta_{1} \right) w^{2} \right] = \left[ \left( a e^{\eta_{0}\lambda} + e^{-\eta_{0}\lambda} \right) \left( 1 + \beta\eta_{1}\lambda^{2} \right) - (a+1) \right] w + \left[ a e^{\eta_{0}\lambda} \left( 2\eta_{1}\beta\lambda + 5\beta \right) + e^{-\eta_{0}\lambda} \left( -2\eta_{1}\beta\lambda + 5\beta \right) - 5\beta(a+1) \right] w^{2}.$$
 (23)

If we divide both sides of equation (23) by  $w^2$ , and neglect the terms in  $\frac{1}{w^2}$ , but not those in  $\frac{1}{w}$  (in some sense we are serching for a "weakly asymptotic" solution), we obtain the following system of two transcendent equations in the unknowns  $\eta_0$  and  $\eta_1$ 

$$-\frac{2}{3}\frac{\zeta^2}{(1+a+\kappa)}\left(\eta_0^2 - 6\beta\eta_0 + 4\beta\eta_1\right) = \left(a\ e^{\eta_0\lambda} + e^{-\eta_0\lambda}\right)\left(1 + \beta\eta_1\lambda^2\right) - (a+1) \tag{24}$$

$$-\frac{2}{3}\frac{\zeta^2}{(1+a+\kappa)}\left(4\eta_0\eta_1 - 3\eta_0^2\right) = a \ e^{\eta_0\lambda}\left(5 + 2\eta_1\lambda\right) + e^{-\eta_0\lambda}\left(5 - 2\eta_1\lambda\right) - 5(a+1),\ (25)$$

where in the second equation we have dropped the common factor  $\beta$ . If we are able to solve the previous system, it is possible to obtain  $\eta_0$  and  $\eta_1$  as functions of the applied electric force  $\zeta$ , and then  $\psi_A(w)$ . Moreover, by using equation (19), one can find  $p_A(w)$ . Henceforth we will indicate as asymptotic solution of the SHE equations the expressions of  $n_A$  and  $p_A$  which can be obtained by means of the approximate solution of (18)-(19) which have been found.

# 6 Discussion of the solution and comparison with numerical results.

An analytical solution of the equations (24)-(25) has turned out to be impossible. Therefore we have limited ourselves to a graphical and numerical analysis. Given a value of the applied electric force  $\zeta$ , the requirement that the functions be integrable in  $[0, +\infty[$  tells us that both  $\eta_0$  and  $\eta_1$  have to assume negative values. In fact, we found a negative solution of the system (24)-(25) in the domain  $[-1,0] \times [-1,0]$  of the  $(\eta_0, \eta_1)$  plane, for all the values of the electric field in the explored range. We used a simple MapleV algorithm in order to find the solutions. In table II we give some of the values we found.

E (V/cm)	$\eta_0$	$\eta_1$
0.0	-1.0	0.0
$1.0 \times 10^{2}$	-0.9999636274	-0.0001493648
$1.0 \times 10^{3}$	-0.9963693066	-0.0148712049
$5.0 \times 10^{3}$	-0.9136708716	-0.3294754506
$1.0 \times 10^{4}$	-0.7162321385	-0.8333494338
$3.0 \times 10^{4}$	-0.2511364699	-0.5681222515
$5.0 \times 10^{4}$	-0.1270766899	-0.2772663271
$7.0 \times 10^{4}$	-0.0780599266	-0.1591756496
$1.0 \times 10^{5}$	-0.0452815087	-0.0850850173

**Table II.** Some values of  $\eta_0$  and  $\eta_1$  as functions of the electric field.

In figures 1, 2 and 3, we compare the asymptotic solution  $(n_A, p_A)$  and the numerical solution  $(n_N, p_N)$  of equations (13)-(14), the latter obtained by a suitable numerical technique (Liotta and Majorana, 1999), for some values of the applied electric field. As is possible to see, the agreement between the numerical and asymptotic solutions is good in all the energy range, despite the obtained asymptotic solution should be good only for high enough energy values (the agreement is obviously very good in this region). We want to observe that for low values of the electric field ( $|\mathbf{E}| \leq 10^3 \text{ V/cm}$ ), instead of formula (19), we use the following expression for  $p_A$ :

$$p_A(w) = \frac{1}{\mu(w+\lambda) + a\mu(w-\lambda) + \kappa\mu(w)} \frac{2}{3} \zeta \frac{[\chi(w)]^{\frac{3}{2}}}{\chi'(w)} \frac{d\psi_A}{dw}.$$
 (26)

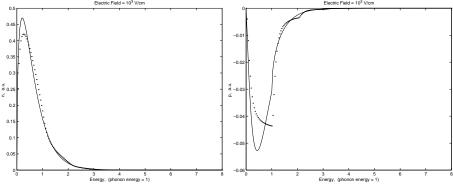


Figure 1: Electric field =  $10^3$  V/cm. n and p versus energy. Dots: numerical solution, continuous line: asymptotic solution. The optical phonon energy is set equal to one.

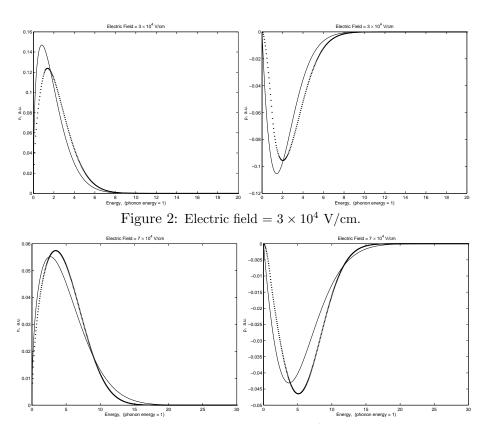


Figure 3: Electric field =  $7 \times 10^4$  V/cm.

This choice is not coherent with the expansion, but allows a better agreement with the numerical solution and puts in evidence a discontinuity in the derivatives at the point  $w = \lambda$  (in dimensional variables  $\varepsilon = \hbar \omega_{op}$ ) due to the term  $\mu(w - \lambda)$ , that is zero for  $0 \le w \le \lambda$ . This term is also present in the original set of equations (13)-(14). Then, such discontinuity is also expected in the solutions.

As a measure of the difference between the numerical and asymptotic solution we can also compute  $V_{as} = \int p_A d\varepsilon / \int n_A d\varepsilon$  and  $V_{num} = \int p_N d\varepsilon / \int n_N d\varepsilon$ , which give, in dimensional units, the electron hydrodynamical velocity. In table III we compare the values we found.

E (V/cm)	$V_{as}(m/sec)$	$V_{num}(m/sec)$
$1.0 \times 10^{2}$	$1.4879 \times 10^3$	$1.4537 \times 10^{3}$
$1.0 \times 10^{3}$	$1.4831 \times 10^4$	$1.3858 \times 10^{4}$
$5.0 \times 10^{3}$	$7.0223 \times 10^4$	$5.1060 \times 10^4$
$1.0 \times 10^{4}$	$6.0652 \times 10^4$	$7.3611 \times 10^4$
$3.0 \times 10^{4}$	$9.8325 \times 10^4$	$9.7714 \times 10^4$
$5.0 \times 10^{4}$	$1.0106 \times 10^5$	$9.9872 \times 10^4$
$7.0 \times 10^{4}$	$9.5124 \times 10^4$	$9.8395 \times 10^{4}$
$1.0 \times 10^{5}$	$8.2528 \times 10^4$	$9.5101 \times 10^4$

**Table III.** Comparison between the electron hydrodynamical velocities calculated by using respectively the asymptotic and numerical solutions.

The behaviour of the hydrodynamical velocity is the typical one when the Kane equation is used (see Tomizawa, 1993, p. 100, fig. 3.11). We do not consider higher values

of the electric field because in this case also the Kane equation becomes inadequate to describe the conduction band, and a full band structure should be used (Vecchi and Rudan, 1998).

### 7 Conclusions and acknowledgments.

We have shown that it is possible to find an "asymptotic solution" of the SHE equation (13)-(14) in which the dependence on the applied electric field is given implicitly through the system of transcendent equations (24)-(25). The solution of the system (24)-(25) can be obtained by using standard numerical techniques. The agreement with the numerical solution is good in all the explored range of applied electric fields.

If we put  $\beta=0$ , we recover the parabolic band case and the asymptotic solution reduces to the asymptotic one already found by Liotta and Majorana (1999) (L-M solution). The L-M solution was used by Anile and Mascali (2000) to obtain a two fluid hydrodynamical model, where the electron population is splitted in two sub-populations: low-energy and high-energy electrons, separated by a threshold energy. In order to close the moment equations relatively to the hot electrons they used a distribution function whose form is directly suggested by the L-M solution, whereas relatively to cold electrons a a standard maximum-entropy distribution function is utilized. A detailed study of the resulting high-energy hydrodynamical model is given in Anile, Liotta and Mascali (2000). Some works about the extension of this model to the case of Kane band, using the asymptotic solution found in this paper, are in progress. A better description of the hot electron population is expected.

The author acknowledges support from Italian CNR (Prog. N.96.03855.CT01), from TMR (Progr. n. ERBFMRXCT970157), from Italian MURST (Prot. n. 9801169828-005) and from "Convenzione quadro Università di Catania-ST Microelectronics".

The author wish also to thank prof. A. M. Anile, prof. A. Majorana and dr. G. Mascali for useful discussions and precious suggestions.

#### References

- [1] Anile, A. M., Liotta, S. F. and Mascali G. (2000), High field fluid dynamical models for the transport of charge carriers in semiconductors, submitted
- [2] Anile, A. M. and Mascali, G. (2000), Theoretical foundations for tail electron hydrodynamical models in semiconductors, to be published on Appl. Math. Lett.
- [3] Cercignani, C. (1987), The Boltzmann equation and its applications, Applied Mathematical Sciences, Vol. 67, Springer-Verlag, New York.
- [4] Ferry, D. K. (1991), Semiconductors, Macmillan Publ. Comp, New York.
- [5] Grad, H. (1958), Principles of the kinetic theory of gases, in: S. Flügge (ed.) Handbuch der Physik, Springer-Verlag, Vol. 12, pp. 205-294.
- [6] Jacoboni, C. and Lugli, P. (1989), The Monte Carlo method for semiconductor device simulation, Springer-Verlag, New York.

- [7] Liotta, S. F. and Majorana, A. (1999), A novel approach to spherical harmonics expansion for electron transport in semiconductors, available at this URL: http://babbage.sissa.it/abs/cond-mat/0003456
- [8] Liotta, S. F. and Struchtrup, H (2000), Moment equations for electrons in semiconductors: comparison of spherical harmonics and full moments, Solid State Electronics, Vol. 44, pp. 95-103.
- [9] Majorana, A. (1998), Spherical-Harmonics type expansion for the Boltzmann equation in semiconductor devices, Le Matematiche, Vol. LIII, pp. 331-344.
- [10] Markowich, P. A., Ringhofer, C. A. and Schmeiser, C. (1990), Semiconductor equations, Springer-Verlag, Wien.
- [11] Rahmat, K., White, J. and Antoniadis, D. A. (1996), Simulation of Semiconductor Devices Using a Galerkin/Spherical Harmonic Expansion Approach to Solving the Coupled Poisson-Boltzmann System, IEEE Trans. Computer-Aided Design, Vol. 15, pp. 1181-96.
- [12] Thorne, K. S. (1981), Relativistic radiative transfer: moment formalism, Mon. Not. R. astr. Soc., Vol. 194, pp. 439-473.
- [13] Tomizawa, K. (1993), Numerical simulation of sub micron semiconductor devices, Artech House, Boston.
- [14] Vecchi, M. C. and Rudan, M. (1998), Modeling electron and hole transport with full-band structure effects by means of the spherical-harmonics expansion of the BTE, IEEE Trans. Elec. Dev., Vol. 45, pp. 230-238.
- [15] Ventura, D., Gnudi, A. and Baccarani, G. (1995), A Deterministic Approach to Solution of the BTE in Semiconductors, Rivista del Nuovo Cimento, Vol. 18, pp. 1-33.